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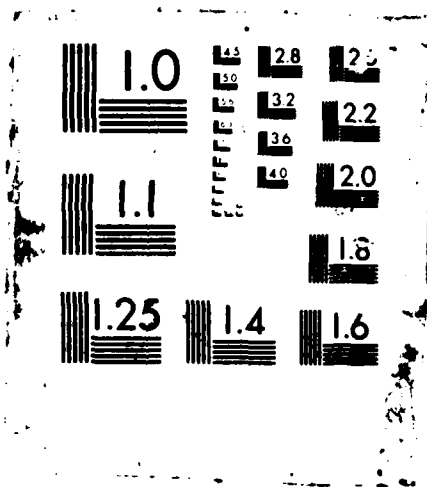AD-A178 361

COMPUTER MODELING AND OPTIMIZATION
OF OBOGS WITH CONTAMINANTS

ANNUAL REPORT
Covering the Period 15 July 1984 - 14 July 1985

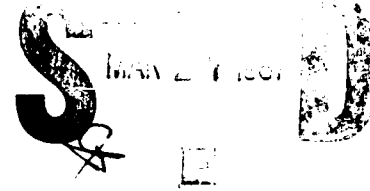Joseph J. Beaman

September 13, 1985

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87 3   26 037

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188
Exp Date Jun 30, 1986

1a REPORT SECURITY CLASSIFICATION	1b RESTRICTIVE MARKINGS
Unclassified	

2a. SECURITY CLASSIFICATION AUTHORITY	3 DISTRIBUTION/AVAILABILITY OF REPORT
	Approved for public release;
2b DECLASSIFICATION/DOWNGRADING SCHEDULE	distribution unlimited

4 PERFORMING ORGANIZATION REPORT NUMBER(S)	5 MONITORING ORGANIZATION REPORT NUMBER(S)

6a NAME OF PERFORMING ORGANIZATION	6b OFFICE SYMBOL (If applicable)	7a NAME OF MONITORING ORGANIZATION
The Univ. of Texas at Austin Mechanical Engineering Dept.		

6c ADDRESS (City, State, and ZIP Code)	7b. ADDRESS (City, State, and ZIP Code)
Austin, Texas	

8a NAME OF FUNDING/SPONSORING ORGANIZATION U.S. Army Medical Research and Development Command	8b OFFICE SYMBOL (If applicable)	9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER
		DAMD17-84-C-4076

8c ADDRESS (City, State, and ZIP Code)	10. SOURCE OF FUNDING NUMBERS			
	PROGRAM ELEMENT NO.	PROJECT NO	TASK NO	WORK UNIT ACCESSION NO
Fort Detrick Frederick, Maryland 21701-5012	62777A	3E1-62777A878	AF	154

11. TITLE (Include Security Classification)

12. PERSONAL AUTHOR(S)

13a TYPE OF REPORT	13b TIME COVERED FROM _____ TO _____	14 DATE OF REPORT (Year, Month, Day)	15 PAGE COUNT

16 SUPPLEMENTARY NOTATION

17	COSATI CODES		18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)
FIELD	GROUP	SUB-GROUP	
06	11		
09	02		

19 ABSTRACT (Continue on reverse if necessary and identify by block number)

20 DISTRIBUTION/AVAILABILITY OF ABSTRACT	21 ABSTRACT SECURITY CLASSIFICATION
☐ UNCLASSIFIED/UNLIMITED ☒ SAME AS RPT ☐ DTIC USERS	Unclassified
22a NAME OF RESPONSIBLE INDIVIDUAL	22b TELEPHONE (Include Area Code)	22c OFFICE SYMBOL
Mrs. Virginia Miller	301/663-7325	SGRD-RMI-S

DD FORM 1473, 84 MAR — 83 APR edition may be used until exhausted
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FOREWORD

Citations of commercial organizations and trade names in this report do not constitute an official Department of the Army endorsemnt or approval of the products or services of these organizations.

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SUMMARY

This report covers the first year of a two year project dealing with the development of an OBOGS computer model to aid in design and specification of these oxygen generation systems for the Army's in-flight, medivac, and field hospital use. A model which predicts the performance of a two bed system for O_2 - N_2 separation has been delivered and installed on the U.S. Army Aeromedical Research Laboratory (USAARL) VAX computer. A model to predict the propagation of contaminants in these beds is currently under development.

STATEMENT OF PROBLEM

The ultimate goal of this research is to insure proper design of molecular sieve oxygen generation systems for the U.S. Army's in-flight, medivac, and field hospital use. Specifically the research involves further development of an OBOGS model to include the effects of contaminants in the feed air. This OBOGS model can be used to optimize and design OBOGS systems with respect to system parameters such as cycle time and bed and valve dimensions.

BACKGROUND

The elimination of the need for liquid oxygen storage for in-flight and portable ground use by means of oxygen generation equipment is an especially attractive goal to the military. Such an accomplishment would not only increase safety, but would relieve the logistics requirements of LOX supply which is costly and can restrict mission durations. Although other means are available, the molecular sieve method of generating enriched oxygen breathing gas is the most feasible for in-flight usage. The molecular sieve system weighs little, and has the potential of high reliability.

A molecular sieve system utilizes the process of physical adsorption to separate air into its components. Although a detailed discussion of adsorptive phenomena is beyond the scope of this report, a brief overview of the process is in order.

Adsorption is the process by which particular types of molecules contained in a liquid or gas are selectively collected onto a solid surface. The term "adsorbent" refers to the collecting material while the "adsorbate" is that material which is collected. In physical adsorption (as opposed to chemical adsorption), Vander Waal's forces create the bonds between adsorbent and adsorbate; thus, the interaction is weak. The solid adsorbent is typically a highly porous, granular material with interior pores of diameters on the order of .4nm, and with the total pore volume approaching 50% of that of the whole particle. Clearly, abundant internal storage space is available in the sieve material.

Adsorptive separation is the process by which the molecular sieve system would separate air into its components and thereby produce an enriched oxygen product gas.

To maintain continuous operation from an adsorption plant, molecular sieve beds must be periodically "regenerated" by a period of desorption in which the adsorbate is removed from the sieve material. There are several ways in which

desorption may be accomplished. "Thermal Swing" involves heating the bed to a temperature at which the adsorptive capacity of the bed material is so low that the adsorbate must leave the molecular sieve internal surfaces. "Pressure swing" creates the same effect by reducing the adsorptive capacity at essentially constant temperature. "Inert purge stripping" removes the adsorbate at constant temperature and pressure by the passage of fluid containing no adsorbate molecules, in which the adsorbate is soluble. "Displacement desorption" occurs when a fluid containing a high concentration of a more strongly adsorbed molecule is passed through the bed. The pressure swing adsorptive cycle, PSA, is of primary concern in this work.

Two important technological developments of recent decades have created the possibility of in-flight and portable air separation systems. Firstly, the domestic development and production of synthetic zeolites, a molecular sieve material, affords the availability of reproducible adsorbents. Secondly, the inception and development of the pressure swing adsorption cycle (PSA) has been found to yield a satisfactory production system.

The PSA process usually employs two or more molecular sieve beds and cycles them in a manner such that a continuous flow of enriched oxygen product gas is attained. Sufficient gas is produced to meet demand and to regenerate exhausted beds via pressure swing method. By use of an appropriate zeolite, oxygen or nitrogen (for fuel tank inerting) can be concentrated to almost any value up to 95% for O_2 and 99.8% for N_2. The product gas can be delivered at normal room temperature and at some nominal pressure as desired. The process cost is basically the cost of air compression for the feed gas.

Traditionally, PSA systems have found applications in industry and have been very large systems which were relatively insensitive to the various rate phenomena of the adsorption process. In the development of a scaled-down system for portable applications, knowledge of transient behavior becomes exceedingly important due to the vastly increased sensitivity of system output to rate phenomena and the requirements of minimal size and weight. Additionally, the effects of potentially harmful contaminants and chemical agents which might be encountered during usage must be better understood.

APPROACH TO THE PROBLEM

CONTAMINANT MODEL

As a first step in the modeling of an OBOGS system, an experimentally verified model of a single bed system containing a zeolite molecular sieve with contaminants in the inlet air is being developed. A model that has been previously developed for two component $O_2 - N_2$ gas mixtures is described in appendix A. Preliminary work with $O_2 - N_2 - CO$ and $O_2 - N_2 - CO_2$ mixtures indicates that a similar model with a third component might be effective for contaminant studies. USAARL is presently conducting single bed experiments with contaminants such as CO_2, CO, C_2H_6O (ethanol), NH_3 (ammonia), C_5H_{12} (pentane), CH_3Br (methyl bromide), NO_2, N_2O_4, O_3 (ozone), CH_4 (methane), CCl_2F_2 (freon 12), acrolein, oil breakdown products, and other battlefield products. These experiments are essentially column breakthrough experiments which will be used to validate the computer model.

Once the dynamics of a single bed are correctly modeled, an overall system model for a two bed system with valves and mixing plenum will be developed. This modeling has been done for $O_2 - N_2$ mixtures. A description is contained in appendix B. A similar model is being developed for contaminant studies.

RESULTS AND CONCLUSIONS

A computer program of the OBOGS model described in appendix B has been delivered and installed on the VAX* computer at USAARL. This program is menu driven for ease of operator use and has REGIS* graphical output for use with VT125* or VT240* graphical terminals. The operator has a choice of output of on-line plotting of oxygen mole fraction or inlet/outlet mass flowrate versus time or off-line plotting of a dynamic simulation of OBOGS for one cycle. The operator can also select and change a variety of geometric and material parameters in order to aid in design studies. Sample inputs and outputs of the program are given in appendix C.

A preliminary 3 component OBOGS has been developed for contaminant studies. Before any further development on this program can continue the results of the experimental single bed data generated by USAARL is necessary. As soon as this data is available, it will be incorporated into a single bed model. Then a two bed OBOGS system model will be developed and experimentally verified.

* Tradename of Digital Equipment Corporation

APPENDIX A

Single Bed Model Technical Description
This article is reprinted from the TRANSACTIONS OF THE ASME, JOURNAL OF
DYNAMIC SYSTEMS, MEASUREMENT, AND CONTROL. The authors are J.J. Beaman,
A.J. Healey, and J. Werlin, Dec. 1983

A Dynamic Model of a Molecular Sieve Bed With Nonlinear and Coupled Isotherms[1]

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A mathematical model of the O_2-N_2 separation process in a molecular sieve bed was developed and experimentally verified. Oxygen and nitrogen breakthrough experiments were performed on a single bed packed with molecular sieve 5A. In these experiments, the bed had initially adsorbed either pure oxygen or nitrogen and then a constant inlet flow of nitrogen or oxygen was switched on the bed. The outlet oxygen mole fraction and mass flowrate were then recorded. This was done at several pressures and flowrates. The model predictions agreed with the experimental data when a linear oxygen isotherm and a nonlinear Langmuir isotherm for nitrogen were used and when these were coupled. The numerical scheme presented in this study to solve the system equations makes efficient use of computation time.

I Introduction

The elimination of the need for liquid oxygen for crew breathing requirements in aircraft is an especially attractive goal. A means of accomplishing this goal is now available through the use of a molecular sieve, OBOGS (On-Board Oxygen Generation System). Molecular sieves are in widespread use industrially [1], but the special problems associated with an OBOGS have led to the need for a reliable computer-based simulation tool that would model the relatively rapid transient response of such systems.

One promising system uses a synthetic zeolite to adsorb nitrogen from engine bleed air, thereby producing oxygen enriched breathing gas. This system uses a "pressure swing" adsorption cycle [2] in order to achieve gas separation. In this cycle, nitrogen is adsorbed from engine bleed air at high pressure (producing oxygen enrichment) and then desorbed and exhausted to the atmosphere at low pressure in order to replenish the sieve material. While large scale industrial systems are in commercial use, size and weight optimized units for airborne applications are still in the development stage.

In order to better understand the operation and scaling laws of the OBOGS, a computer model of this system has been developed. As a first step in this development, a model of a single molecular sieve bed with identified parameters is needed. This paper addresses the formulation and verification of such a model for predicting the transient response of gas flow rate and gas concentration at the bed outlet to sudden changes in gas composition at the bed inlet.

Previous work in this area has treated the diffusion process to be instantaneous [3, 4] or has considered one component at the trace level [5]. This work considers a complete "washout" of one gas type using another. In other words, mole fractions at the inlet undergo step changes from 0 to 1 and vice versa, while the bed back-pressure and inlet flows are essentially constant.

II Theoretical Model

Figure 1 shows a schematic of the experimental single bed which was used to validate the molecular sieve bed model, where component A is oxygen, B is nitrogen, x is oxygen mole
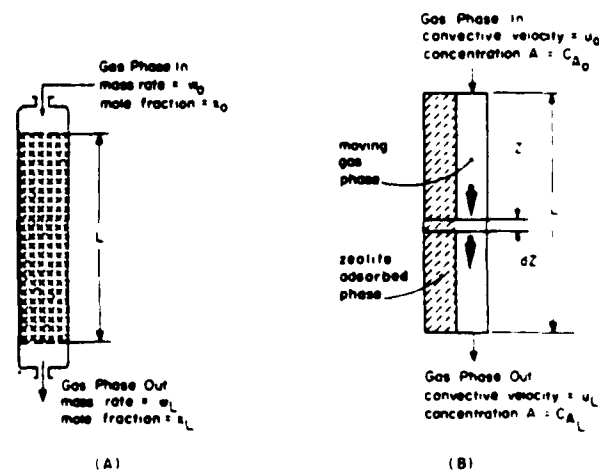
Fig. 1   Single molecular sieve bed

APPENDIX A

sieve bed is 25.4 cm × 14.0 cm × 14.5 cm. loaded with 3.8 Kg of Linde 5A sorbent screened through a 20 to 40 meshes/in. This corresponds to zeolite particles 340 to 833 microns in diameter. The void fraction of the bed is approximately $\epsilon = 0.36$. All experiments were run at room temperature of 25°C.

On the supply side of the bed were cylinders of pressurized O_2 and N_2. Inflow was regulated by standard reducing valves and two variable orifice needle valves, each of which controlled the flowrate out of one cylinder only. A three-way tap valve was used to produce the step change in gas composition. Pressure transducers were located at the bed inlet and outlet. These transducers were located at the bed inlet and outlet. These transducers served as a check on the isobaric assumption. The amount of pressure drop across the bed was on the order of 3 percent of inlet pressure. A mass flowmeter was located just beyond the bed outlet to measure outflow. Outlet O_2 mole fraction was measured with a respiratory mass spectrometer. Experimental data were taken for various flowrates at four different outlet pressures: ½ atm, 1 atm, 2 atm, and 3 atm. A hypobaric chamber was employed for the ½ atm test, while a hyperbaric chamber served as the plenum chamber for the 2 and 3 atm tests. For more information on the tests see Werlin [17].

Figure 3 shows the general nature of the oxygen and nitrogen "breakthrough" experiments where the symbols refer to experimental data. From 0 to 16 seconds an oxygen breakthrough is shown. As seen in this figure, the outlet mass flowrate rises to approximately twice the inlet flowrate and slowly trails off to its equilibrium value. The outlet mole fraction concentration starts at pure nitrogen and rises slowly to pure oxygen. At 16 seconds, the inlet flow is suddenly switched to pure nitrogen. As this point the outlet flow drops almost immediately, is constant for a while, and, finally it rises back to its equilibrium value as the concentration "front" propagates through the bed. The concentration time profile is much sharper than the oxygen breakthrough case, and at approximately 24 seconds the oxygen has been completely washed out.

This general behavior can be explained by the fact that 5A sorbent has a larger affinity for nitrogen than oxygen, so, when oxygen is washed out, more nitrogen is adsorbed than oxygen is given up. Therefore, the flowrate will be reduced ahead of the concentration front. The concentration front remains sharp due to the fact that the velocity ahead of the front is lower than that behind it.

For oxygen breakthrough, the effect is reversed. In this case, more nitrogen is desorbed than oxygen is adsorbed. There is a higher flowrate ahead of the front, and oxygen and nitrogen will tend to be convected away from this region, leading to a broader concentration front.

IV Identification of Model Parameters and Comparison With Experimental Data

Effect of Model Parameters. A quantitative assessment of the effect of the model parameters on the characteristic flowrate and mole fraction time plots can be made by writing (5) through (8) in nondimensional form as

$$\frac{\partial \omega}{\partial \zeta} + 1 = g \tag{24}$$

$$\frac{\partial(\omega x)}{\partial \zeta} + x = g_A \tag{25}$$

$$\frac{\partial \eta}{\partial \tau} + g = 1 \tag{26}$$

$$\frac{\partial \eta_A}{\partial \tau} + g_A = x \tag{27}$$

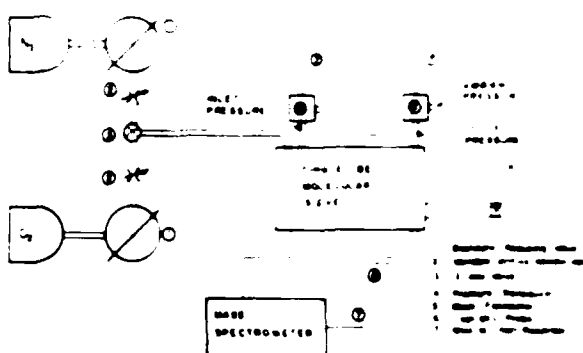Fig. 2 Experimental apparatus

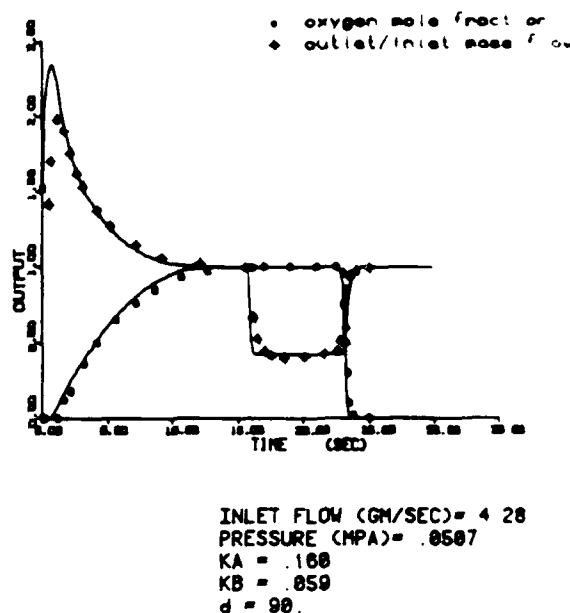- oxygen mole fraction
- outlet/inlet mass flow

INLET FLOW (GM/SEC)= 4.28
PRESSURE (MPA)= .0507
KA = .168
KB = .059
d = 90.

Fig. 3 ½ Atmosphere breakthrough data and simulation – linear isotherms

where

$\omega = u/u_0$, u_0 = inlet convective velocity, $\zeta = \beta Z/u_0$,
$\eta = n/n_0$, n_i = initial adsorbed phase concentration,
$\eta_A = n_A/n_i$, $\tau = tK_A d$, $x = C_A/C$, $g = \gamma/C$, and
$g_A = \gamma_A/C$.

The single component isotherms of (18) and (19) can be expressed as

$$g_A^0 = n_A^0 \tag{28a}$$

$$g^0 = (1 - \mu)\eta_A^0/(1 - \alpha\eta_A^0) \tag{28b}$$

where $\mu = 1 - K_B/K_A$ and $\alpha = n_0/b$. The ideal adsorption method is then used to couple these isotherms. For a nitrogen breakthrough, the initial and boundary conditions become

$$\omega(0,\tau) = 1$$
$$x(0,\tau) = 0$$
$$\eta(\zeta,0) = 1$$
$$\eta_A(\zeta,0) = 1$$

Equations (24) through (28) with these conditions can then be solved numerically, as discussed previously, for values of the two parameters μ and α. These simulations indicate that the nondimensional distance down the bed is related to nondimensional travel time by

$$\zeta = (1 - \mu + \alpha)(\tau_{50} - 0.70) \tag{29}$$

where τ_{50} is the nondimensional time for the outlet oxygen

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APPENDIX A

Table 1 Nitrogen breakthrough experimental results

P Bed pressure MPA	W_0 Inlet flowrate g/s	W_d Mass flow droop W'_{min}/W'_0	t_{50} time to 50% s
0.0507	3.21	0.41	9.40
0.0507	4.28	0.43	7.35
0.100	4.28	0.50	10.7
0.100	8.40	0.52	5.80
0.204	6.53	0.63	15.0
0.203	8.46	0.65	12.2
0.303	6.42	0.70	19.5
0.303	8.56	0.72	14.9

mole fraction to drop to 0.5 or 50 percent. This linear relation arises due to the fact that the outlet velocity drops to a value

$$\omega_d = 1 - \mu + \alpha \text{ for } 0 < \mu - \alpha < 1, \tag{30}$$

where ω_d is the droop velocity as determined by simulation and seen in Fig. 3 for $t > 16$ seconds. This velocity remains relatively constant for a time determined by the length of the bed. (The 0.70 in the (30) above comes from an intrinsic exponential time constant in the process, i.e., $e^{-.70} = 50$ percent.) For a given value of τ_{50}, the length at which the mole fraction "front" is 50 percent would be approximately: length = droop velocity x time to 50 percent which is the interpretation of equation (29).

Identification of Model Parameters. The values of K_A, K_B, b, and d can be effectively found by using breakthrough data and the results of the preceding section. The steps to obtain these parameters from a nitrogen breakthrough are:

(1) Obtain values of $\mu - \alpha$ from flowrate droop data, i.e., $\mu - \alpha = 1 - \omega_d$ for at least two different bed pressures. This allows calculation of μ and α.

(2) Use (29) to obtain a value of K_A from the time for 50 percent breakthrough. The value of d is superfluous to the calculation since $\beta = d(1 - \epsilon)/\epsilon$ and $\tau_{50} >> 0.70$ for the system under study. Using these two relations, (29) yields

$$K_A = L(1 - \epsilon)/u_0(1 - \mu + \alpha)\epsilon t_{50}$$

(3) Use $K_B = (1 - \mu)K_A$ to calculate K_B.

(4) From dimensional analysis, one sees that x is a function of ζ and τ and therefore

$$\frac{\partial x}{\partial t} = \frac{\partial x}{\partial \tau} \frac{\partial \tau}{\partial t} = K_A d \frac{\partial x}{\partial \tau}$$

This implies that the slope or tangent of $x(L, t)$ is directly proportional to d. This fact can then be used to adjust d to match the mole fraction slope.

This resulting identification procedure can be checked by comparing oxygen breakthrough data and additional nitrogen breakthrough data to simulation predictions.

In Table 1, the experimental results of nitrogen breakthrough experiments of ½, 1, 2, and 3 atmospheres are presented. Since more than the minimum two different pressures are available (theoretically all droop data should be identical at the same pressure), a least squares fit of all the droop data was used to find values of μ and α. Note $\omega_d = W_d M_{N_2}/M_{O_2}$ where $M_{N_2} = 28$ for nitrogen and $M_{O_2} = 32$ for oxygen. A value of K_A is then found from step 2 as

$$K_A = L(1 - \epsilon)\rho_0 A_s/W_0(1 - \mu + \alpha)t_{50}$$

where ρ_0 is the bed inlet gas density. From step 3, $K_B = (1 - \mu)K_A$. Using slope adjustment as indicated in step 4, the mass transfer coefficient d was set at a value of 90 s^{-1} at 1/2 atm and $W_0 = 4.28$ gm/s. This value is adjusted for pressure and flow rate by using a correlation due to Lightfoot [18] which indicates that d is proportional to $W^{.49}/P$ where W is mass flowrate and P is pressure. In any case, the value of d did not
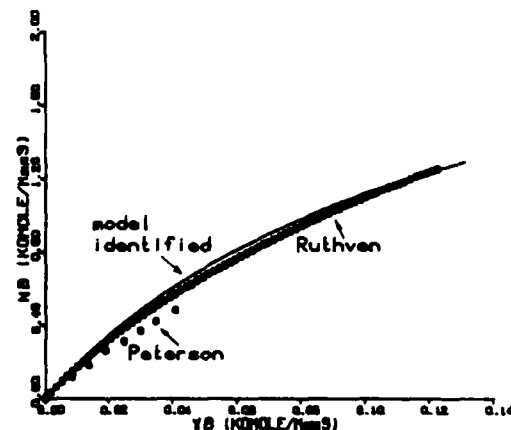

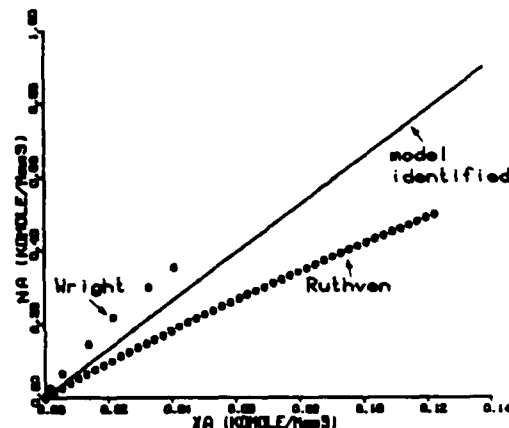**Fig. 4 Nitrogen isotherm**

Fig. 5 Oxygen isotherm

have a large effect on the characteristic response. The result of this identification procedure gave the following parameter identification:

$K_A = 0.153$		$\sigma_{KA} = 0.0185$	
$K_B = 0.0506$		$\sigma_{AB} = 0.00611$	
$b = 2.59$		$\sigma_b = 0.31$	

The σ's are the predicted standard deviations of the parameters.

As a validation of this procedure for identifying isotherm parameters a comparison with published isotherms and correlations is shown in Figs. 4 and 5. Plotted in Fig. 4 are the nitrogen isotherm data of Peterson [19], the correlation of Ruthven [10] based on a statistical thermodynamics model, and the Langmuir isotherm identified in this work. In Fig. 5, the oxygen isotherm data of Wright [20], the correlation of Ruthven [10], and the linear isotherm identified in this work are presented. The match between the nitrogen data and the model isotherm is excellent. The difference in the two sets of oxygen data in Fig. 5 is probably due to the relatively small amount of oxygen absorbed on zeolite 5A, which requires a very accurate gravimetric measurement. The model identified isotherm bisects both sets of given oxygen data.

Comparison of Simulation and Experiment. Comparisons of the model, using the identified parameters, with the experimental data are shown in Fig. 3 and in Figs. 6 through 10. Shown in Fig. 3 are the data and simulation for bed pressure at ½ atm for *both* oxygen and nitrogen with linear isotherms. As can be seen here for low pressure, a linear isotherm is adequate for predicting the time responses. The same values of K_A and K_B were then used for the 3 at-
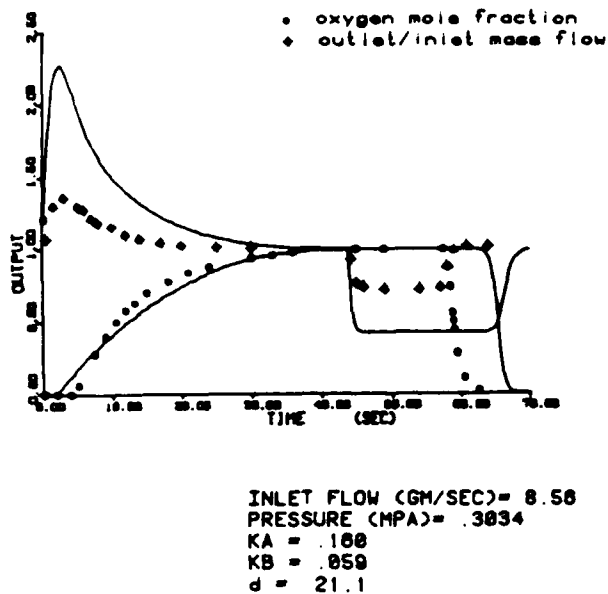
12

INLET FLOW (GM/SEC)= 8.56
PRESSURE (MPA)= .3034
KA = .168
KB = .059
d = 21.1

Fig. 6 3 Atmosphere breakthrough data and simulation – linear isotherms
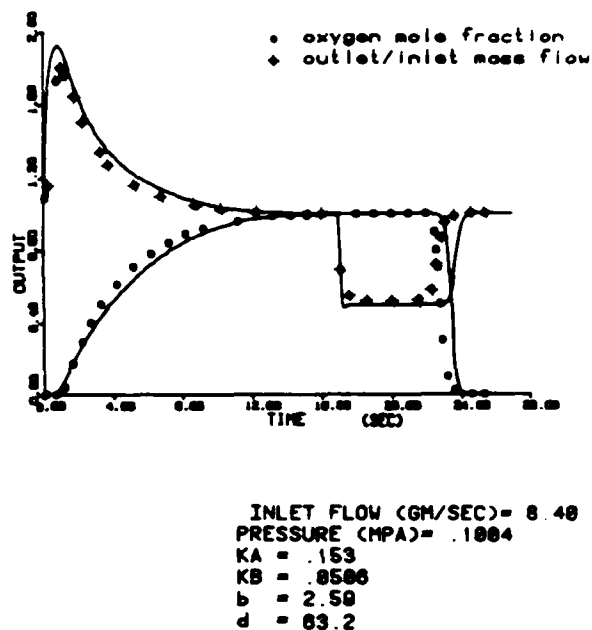
INLET FLOW (GM/SEC)= 8.48
PRESSURE (MPA)= .1004
KA = .153
KB = .0506
b = 2.59
d = 83.2

Fig. 8 1 Atmosphere breakthrough data and simulation – nonlinear coupled isotherms

INLET FLOW (GM/SEC)= 4.28
PRESSURE (MPA)= .0507
KA = .153
KB = .0506
b = 2.59
d = 90.

Fig. 7 '1 Atmosphere breakthrough data and simulation – nonlinear coupled isotherms

INLET FLOW (GM/SEC)= 8.53
PRESSURE (MPA)= .2041
KA = .153
KB = .0506
b = 2.59
d = 27.5
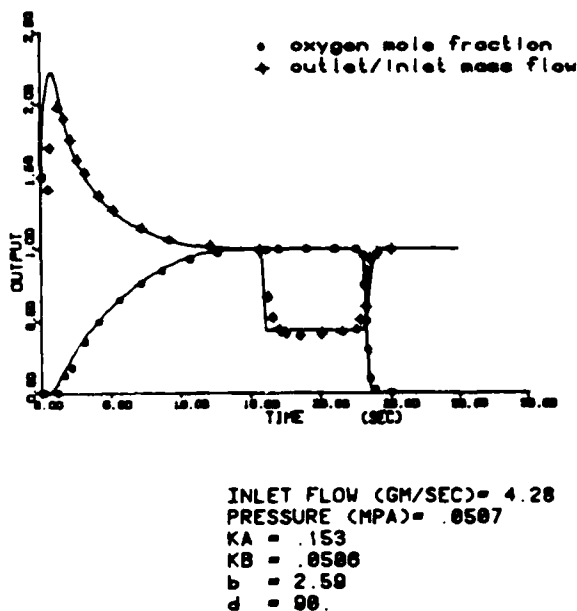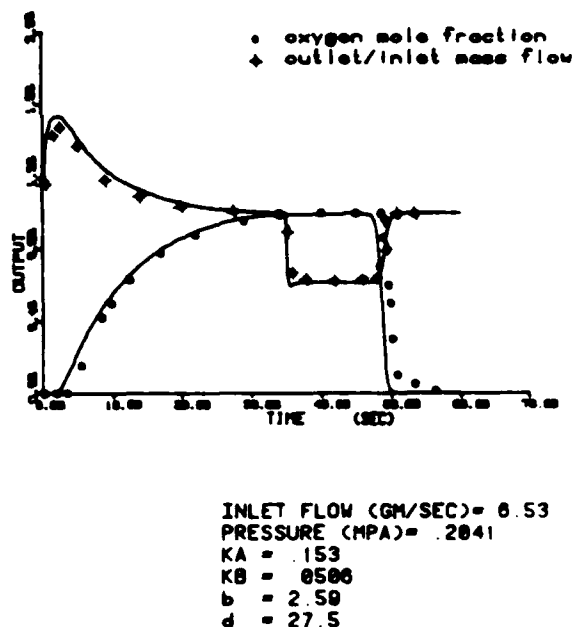
Fig. 9 2 Atmosphere breakthrough data and simulation – nonlinear coupled isotherms

mosphere data, with the results of this simulation shown in Fig. 6. As can be seen, the match with experimental data is very poor. This indicates nonlinear isotherms are necessary.

Comparisons of the model using the nonlinear nitrogen isotherm with the experimental data are presented in Figs. 7 through 10., As seen in these figures, the data match has been greatly improved over the linear parameter model. Discrepancies between model and experiment can be attributed to experimental error and inaccurately assumed isotherms. The data indicate that a nonlinear oxygen isotherm may be appropriate, but this improvement is left for future work.

V Conclusions

A dynamic model of the $O_2 - N_2$ isobaric breakthrough process in a molecular sieve bed was developed and validated experimentally. This model includes nonlinear and coupled isotherms. The proposed model accurately predicts the outlet mole fraction and outlet mass flow. In addition, isotherms for oxygen and nitrogen were identified which are in agreement with previously obtained isotherms.

This model is presently being used in an overall system model for a pressure swing adsorption process to generate oxygen from aircraft engine bleed air.

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• oxygen mole fraction
♦ outlet/inlet mass flow

INLET FLOW (GM/SEC)= 8.56
PRESSURE (MPA)= .3034
KA = .153
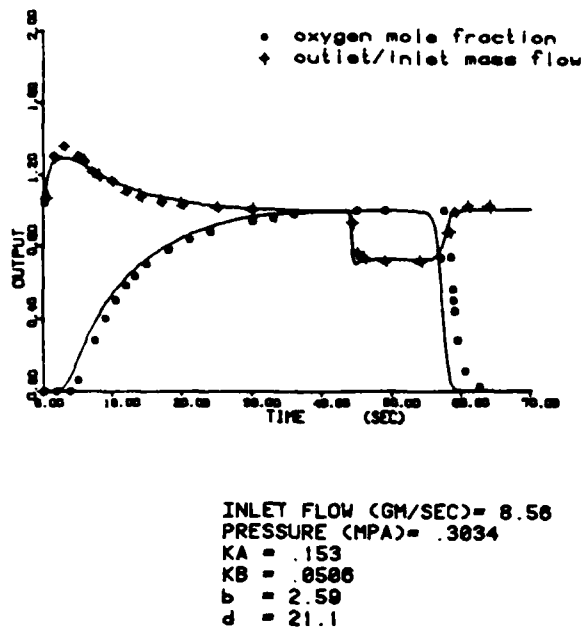KB = .0506
b = 2.59
d = 21.1

Fig. 10   3 Atmosphere breakthrough data and simulation — nonlinear coupled isotherms

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DYNAMIC SYSTEMS, MEASUREMENT, AND CONTROL. The author is J.J. Beaman.

A Dynamic Model of a Pressure Swing Oxygen Generation System[1]

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A full system model for oxygen generation from a pressure swing adsorption process is developed. The system under study has two zeolite packed molecular sieve beds which are cycled with high and low pressure in order to produce oxygen enriched air. These On-Board Oxygen Generation Systems (OBOGS) are to be used for the generation of aircraft crew breathing requirements. These units are much smaller in scale than present industrial systems and are called on to respond to variable demand. These special requirements have led to a reliable computer-based model to simulate the relatively fast transient performance of OBOGS. Besides the two zeolite beds, the system consists of a rotary valve used to cycle the beds, purge orifice, and breathing plenum. The computerized model predictions compare favorably with experiment. The model is presently being used in design and control synthesis studies.

1 Introduction

As mentioned in [1], a promising system for generating breathing oxygen for aircraft crew uses a synthetic zeolite material to physically adsorb nitrogen from engine bleed air. One such system is based on a "pressure swing adsorption cycle" in which nitrogen is adsorbed at high pressure and then desorbed at and exhausted to low pressure. The total process produces oxygen enrichment of air in a cyclical fashion. As a first step in the modeling of such systems, an experimentally verified model of a single bed system containing a zeolite molecular sieve bed was developed in [1]. The model developed in [1] provides predictions of the bed's transient outlet flowrate and mole fraction for a given inflow and mole fraction. The model was tested for pressures from 1/2 to 3 atmospheres and inlet mass flowrates of 3.21 gm/s to 8.56 gm/s.

Related work in this area can be found in Turnock and Kadlec [2] who study the sorption of nitrogen and methane with pressure swing adsorption. Wright et al. [3] develop a system model for a thermal swing adsorption cycle for CO_2 removal. Chan et al. [4] develop an equilibrium theory for pressure swing adsorption. Fernandez and Kenney [5] study a single column pressure swing separation of oxygen and nitrogen. Chihara and Suzuki [6] develop a nonisothermal pressure swing adsorption model. Carter [7] studies pressure swing adsorption for air drying.

Molecular sieve zeolite separation processes are in widespread use industrially, but OBOGS (acronym for On-Board Oxygen Generation System) units are much smaller in scale and are called on to respond to a much more variable demand as determined by the aircraft crew's breathing requirements. These special requirements have led to the need for a reliable computer-based simulation tool that would model the relatively rapid transient response in OBOGS. This model will be useful for both design modification and control development.

2 Description of System

Shown in Fig. 1 is a schematic of a two bed OBOGS developed by Bendix Corporation for use in military aircraft. The object of the system model is to simulate the transient oxygen concentration delivered to the pilot given the pilot's (time varying) breathing mass flowrate. This is accomplished by mathematically modeling the rotary valve, purge orifice, the two zeolite beds, and the breathing plenum, and coupling these separate models into an overall system model.

The pressure swing adsorption cyclic operation of the beds can be described as:

1. The inlet of bed 1 is supplied air at supply pressure through the rotary valve, while bed 2 is being purged to exhaust pressure through the valve. During this stage breathing flow is obtained from bed 1.

2. As the rotary valve turns, the inlet of bed 1 is switched to exhaust pressure and the inlet of bed 2 is switched to supply pressure. During an initial transition stage, the pressure in bed 1, P_1, is still higher than the pressure in bed 2, P_2. In this case, there is flow out of both sides of bed 1 and into both sides of bed 2. Breathing flow will come from the higher pressure bed 1.

3. As the pressure drops in bed 1 due to outflow and builds in bed 2 due to inflow, P_2 will become greater than P_1. This is the identical case of (1) above, but with bed 2 the higher pressure side. The stages 1, 2, and 3 above describe 1/2 of a production cycle. The other half cycle is symmetric to the first half cycle.

The components of the system are the zeolite molecular sieve beds, rotary valve, bypass or purge valve between the two beds, and the breathing plenum. These components are modeled as discussed below.
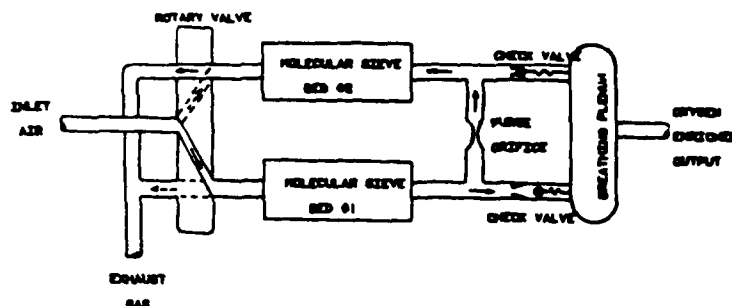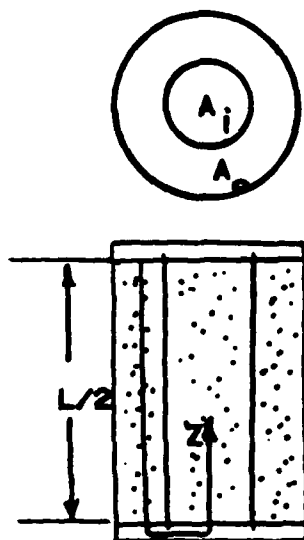
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Fig. 1 Schematic of OBOGS

Fig. 2 Concentric zeolite bed

2.1 Zeolite Bed Model. Concentric beds were used in the experimental study and one is depicted in Fig. 2. As discussed in [1], if we assume one dimensional flow, negligible axial diffusion, diffusion into the zeolite described with a mass transfer coefficient, convective terms dominate temporal changes in the free stream concentration, and isobaric beds (the pressure drop across the beds is small), the oxygen/nitrogen adsorption in the beds can be modeled as

$$\frac{\partial(uA)}{\partial z} = A\beta(\gamma/C - 1) \tag{1}$$

$$\frac{\partial(yA)}{\partial z} = A\beta(\gamma_A - y/u) \tag{2}$$

$$\frac{\partial n}{\partial t} = -d(\gamma - C) \tag{3}$$

$$\frac{\partial n_A}{\partial t} = -d(\gamma_A - C_A) \tag{4}$$

where

A = bed cross-sectional area
d = overall mass transfer coefficient
$\beta = d(1 - \epsilon)/\epsilon$; ϵ = void fraction of gas volume to total volume
$C = C_A + C_B$ total gas phase concentration
C_A = oxygen gas phase concentration
$\gamma = \gamma_A + \gamma_B$ total interfacial concentration
γ_A = oxygen interfacial concentration
u = convective velocity
$n = n_A + n_B$ total adsorbed phase concentration
n_A = oxygen adsorbed phase concentration
$y = uC_A$ convective oxygen flux

Due to the relatively fast heat transfer, it was observed that

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Nomenclature

A = bed cross-sectional area, m^2
A_d = orifice area, m^2
A_i = inner annulus area, m^2
A_o = outer annulus area, m^2
C = gas concentration, kgmole/m^3
C_d = valve discharge coefficient
C_p = breathing plenum gas concentration, kgmole/m^3
d = total mass transfer coefficient, 1/s
k = ratio of specific heats
L = bed length, m
$\dot{M}$ = average molecular weight of gas in plenum, kg/kgmole
n = adsorbed phase concentration, kgmole/m^3
P_0, P_1, P_2, P_3 = supply, Bed 1, Bed 2, exhaust pressures, (N/m^2)
Q = volume flowrate, m^3/s
t = time, s
u = convective velocity, m/s
$\dot{w}$ = mass flowrate, kg/s
y = molecular flux of oxygen, kgmole/m^2·s

z = bed distance, m
β = $d(1 - \epsilon)/\epsilon$ (1/s)
γ = interfacial concentration, kgmole/m^3
Δt = time step, s
Δz = space lump, m
ϵ = void fraction
A = denotes property of oxygen
B = denotes property of nitrogen
BR = denotes breathing property
i = space index
j = time index
L = denotes property at $z = L$
P = denotes purge orifice property
0 = denotes property at $z = 0$
1 = denotes bed 1 property
2 = denotes bed 2 property

Superscripts

$-$ = denotes property just before $z = L/2$
$+$ = denotes property just after $z = L/2$

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the experimental beds remained at essentially constant temperature during a cycle even though the adsorption process is not intrinsically isothermal. A more detailed study of the thermal properties of the system is the subject of ongoing research. In the isothermal case, γ_A and γ_B, the interfacial concentrations of oxygen and nitrogen, respectively, are related to n_A and n_B, the adsorbed oxygen and nitrogen concentrations, by the equilibrium adsorption isotherms [8]. As discussed in [1], these isotherms can be expressed as

$$\gamma_A = \gamma_A(n_A, n_B) \qquad (5a)$$

$$\gamma_B = \gamma_B(n_A, n_B) \qquad (5b)$$

for nonlinear coupled isotherms. The pure component isotherms were identified as

$$\gamma_A^* = K_A n_A^* \qquad (6a)$$

$$\gamma_B^* = K_B n_B^*(1 - n_B^*/b) \qquad (6b)$$

with $K_A = 0.153$ kgmole gas phase/kgmole adsorbed phase, $K_B = 0.0506$ kgmole gas phase/kgmole adsorbed phase, and $b = 2.59$ kgmole adsorbed phase. The coupling is predicted by using an ideal adsorption method [1].

The diffusion coefficient d was empirically chosen as 200 1 s in order to best match the data. This value is higher than the values identified in [1]. This is probably due to the high velocities in the beds during exhaust and initial intake of air.

2.2 Valve Model. The orifices of the rotary valve and the purge orifice are modeled as standard compressible flow pneumatic orifices as described in [9]. The basic equation for the flow of a gas through an orifice is of the following form

$$W = C_d A_o f\left(P_u, T_u, \frac{P_d}{P_u}\right) \qquad (7)$$

where

W = mass flowrate
A_o is orifice area
C_d is a dimensionless discharge coefficient
T_u is upstream stagnation temperature
P_u is upstream stagnation pressure
P_d is downstream pressure
f is a function of P_u, T_u, and P_d/P_u.

For pressure ratios P_d/P_u greater than the choked flow ratio and less than 1, the function f can be expressed as

$$f = C_1 \frac{P_u}{T_u^{1/2}} (P_d/P_u)^{1/k}(1 - (P_d/P_u)^{(k-1)/k})^{1/2}; \qquad (8)$$

for pressure ratios less than the choked flow ratio,

$$f = C_2 \frac{P_u}{T_u^{1/2}},$$

where C_1 and C_2 are functions of k, the ratio of specific heats, and the gas constant. These parameters are taken as constants for this study. For the rotary valve the orifice areas are cyclic functions of the rotation angle of the valve. The discharge coefficients were chosen between values of 0.6 and 1, in order to best match the measured experimental flow.

2.3 The Breathing Plenum. The breathing plenum is modeled as an ideal isobaric two stage mixing chamber. The transfer function between inlet mole fraction and outlet mole fraction can be expressed as

$$\frac{x_o}{x_i} = \frac{1}{(\tau s + 1)^2} \qquad (9)$$

where

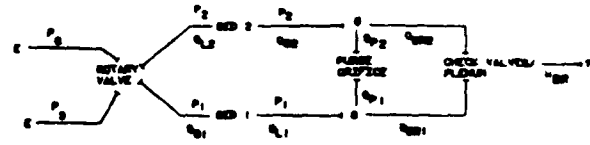$$\tau = \frac{C_p V_{BR} \bar{M}}{W_{BR}}$$

Fig. 3 Conceptual bond graph of system

W_{BR} is breathing mass flowrate, C_p is the plenum molecular concentration, V_{BR} is approximately half of the plenum volume, $\bar{M}$ is an average molecular weight. In deriving these equations the following assumptions have been made:

1. The plenum remains at approximately constant pressure and therefore constant C_p. This is not strictly true as breathing oxygen is being switched between the beds, but for our prototype system this assumption is reasonable.

2. The molecular flux into and out of the plenum can be found approximately from the mass flowrate and an average molecular weight. This assumption is quite reasonable for oxygen and nitrogen since their individual molecular weights do not differ substantially.

3. The mixing volumes for the two idealized chambers are equal and can be found from half the plenum volume plus a correction for mixing in the piping.

3 Solution Technique

3.1 Causal Considerations. The overall system model can be depicted by the word bond graph [10] shown in Fig. 3. Besides the physical interconnections, the graph also indicates the important causal relationships in the system model. The causality shown in the graph can be read as:

1. Pressures P_0 and P_1 are supplied as inputs to the rotary valve while the valve determines the flowrate Q_{01} from these two pressures.

2. P_1 is determined from bed 1 which has inputs the flow Q_{01} and the flow Q_{L1}.

3. Pressures P_1 and P_2 are the inputs to the purge valve and the valve supplies the flowrates Q_{P1} and Q_{P2} to the system. Q_{BR1} and Q_{BR2} are determined by the breathing flow and bed pressures in the check valve/plenum system as described in the next section.

4. P_2 is determined by bed 2 which has inputs the flows Q_{02} and Q_{L2}.

5. Q_{L2} is determined by the rotary valve with inputs to the valve of P_2 and P_3.

In addition to these causal statements, the spatial molecular concentration of the two gases in the beds is determined in the direction of the flowrate i.e., the concentration must be determined from upstream conditions. This will be discussed more thoroughly in the next section.

The causality described above and shown on the graph is integral causality for the beds if they are treated as capacitive fields [11] or mass storage devices. Using other causal arrangements is possible but will result in complicated and computationally time consuming iteration.

3.2 Solution Algorithm. Given input supply pressures P_0 and P_1, breathing flow W_{BR}, and initial adsorbed phase concentrations $n(z,0)$ and $n_A(z,0)$ in the two beds, the system equations can be solved as a boundary value problem in space and a marching problem in time. The solution technique consists of:

(i) Given $n(z,0)$ and $n_A(z,0)$, the interfacial gas phase concentrations $\gamma(z,0)$ and $\gamma_A(z,0)$ can be calculated from the equilibrium isotherms (5). Equation (1) can then be integrated along the entire length of each bed as

$$(Q_i - Q_0 + A_i \beta L/2 + A_0 \beta L/2)C$$

$$= A_0 \beta \int_0^{l/2} \gamma dz + A_i \beta \int_{l/2}^{l} \gamma dz. \qquad (10)$$
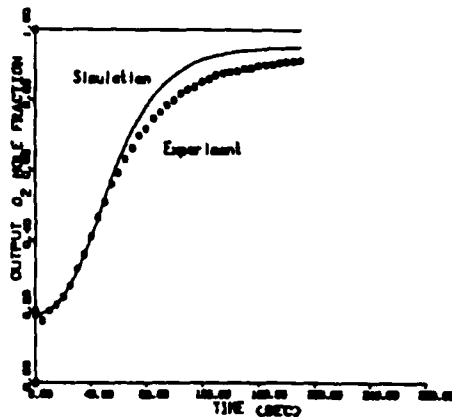
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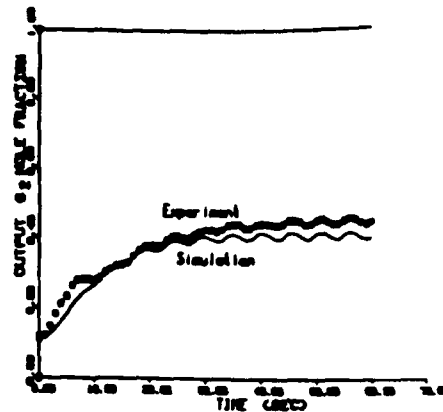Fig. 4 Oxygen mole fraction versus time (10 (lit/min) breathing flow)

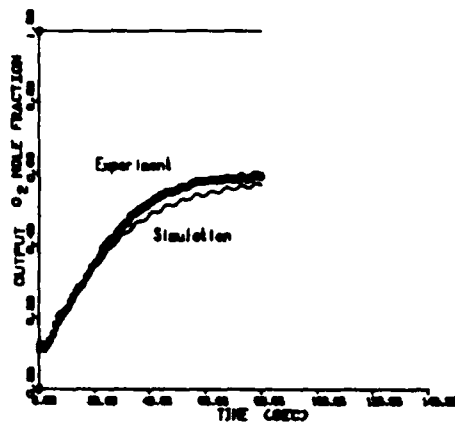Fig. 6 Oxygen mole fraction versus time (50 (lit/min) breathing flow)

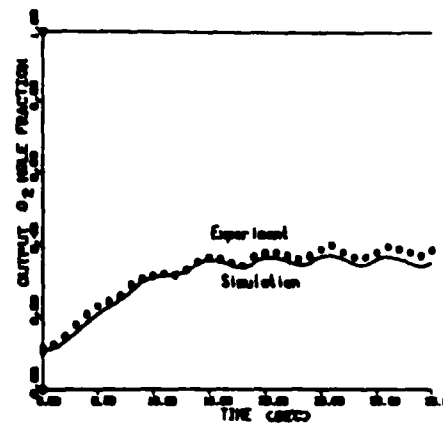Fig. 5 Oxygen mole fraction versus time (30 (lit/min) breathing flow)

Fig. 7 Oxygen mole fraction versus time (70 (lit/min) breathing flow)

For bed 1, $Q_0 = Q_{01}(P_0, P_1)$ where P_1 is proportional to C_1, the gas phase concentration in bed 1, for isothermal beds and assuming a perfect gas, and $Q_L = Q_L (P_1, P_2) - Q_{BR1}$ where P_2 is proportional to C_2, the gas concentration in bed 2 and Q_{BR} accounts for the volume flow out of bed 1 due to crew breathing. For product flow out of bed 1, Q_{BR1} is proportional to W_{BR} for an isobaric and isothermal phenum. For bed 2, $Q_0 = Q_{02}(P_1, P_2) - Q_{BR2}$ and $Q_L = Q_{L2}(P_2, P_3)$ where Q_{BR2} accounts for breathing flow out of bed 2. Note that either Q_{BR1} or Q_{BR2} will be zero depending on which bed had the lower pressure. Equation (10) written out for both beds represents two coupled nonlinear algebraic equations for the two unknowns C_1 and C_2. These equations can be solved by an iteration procedure consisting of (1) assuming concentration C_2 and solving the resultant single nonlinear algebraic equation for C_1 using a modified false position algorithm, (2) using this value of C_1 to calculate a new value of C_2, (3) iterate until the solution procedure converges. Convergence of this procedure requires on the order of three to four iterations. The integrations involved in (10) are performed numerically by a trapezoidal rule, and are only done once per time step. This iteration procedure amounts to a solution of the boundary value problem in the system.

(ii) Spatially integrate equation (1) numerically as

$$u = u_{-1} + \beta(\gamma_i + \gamma_{-1})/2C - \beta\Delta z, \qquad (11)$$

where i is the index for the space dimension, $z = i\Delta z$, and Δz is the space lump size. This integration is done in two steps from 0 to $L/2$ and then from $L/2$ to L with condition $u(z^*) = A(z-u(z^-))/A(z^+)$ at $z = L/2$ to account for the area

change in the outer annulus and inner cylinder of the bed. Note that the starting velocity $u_0 = Q_0/A(0)$ is known from step (i).

(iii) Using the velocity distribution calculated in (ii), equation (2) is a first order linear ordinary differential equation in space for fixed time. Approximate the velocity u and the interfacial concentration γ_A over a space lump as

$$u = r_0 + r_1 z$$

$$(i-1)\Delta z < z < i\Delta z$$

$$\gamma_A = r_2 + r_3 z$$

where

$$r_0 = u_{i-1}, \quad r_1 = (u_i - u_{i-1})/\Delta z$$

$$r_2 = \gamma_{Ai-1}, \quad r_3 = (\gamma_{Ai} - \gamma_{Ai-1})/\Delta z$$

Using these approximations, equation (2) can be integrated in closed form as shown in [1] The direction of the integration will always be in the direction of the velocity flow. Which, as described in Section 2, might be (1) flow in one side of the bed and out the other, (2) flow into both sides of the bed, or (3) flow out of both sides of the bed. In cases (2) and (3), there will be at least one point in the bed that has zero flow. As the velocity in the bed is found as described in (ii) above, the point of zero velocity is stored. For case (1), the integration will proceed in the direction of flow; for case (2) the integration will proceed from the sides of the bed to the point of zero flow; and for case (3) the integration will start at the point of zero velocity and proceed out the two sides. Although physically possible, multiple points of zero flow will not occur
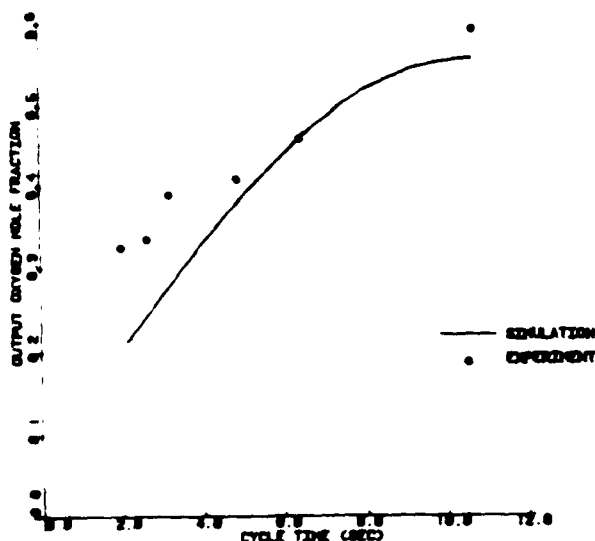
Fig. 8 Oxygen mole fraction versus cycle time (30 (lit/min) breathing flow)

Fig. 9 Effect of reducing active sieve volume

in normal operation of OBOGS and this case is not included at present in the computerized solution.

The ability to solve equation (2) in closed form is an important numerical result. The oxygen profiles in the beds can be very steep, and if a completely numerical procedure is applied to (2), it will require small increments for Δz in order to be stable and accurate. This will result in very long computation times even on a high speed computer.

(ii) Equations (3) and (4) are then integrated in time via a simple Euler method as

$$n_{i,j} = n_{i,j-1} - d(\gamma_i - C)\Delta t \qquad (12)$$

$$n_{A_i,j} = n_{A_i,j-1} - d(\gamma_{A_i} - C_{A_i})\Delta t \qquad (13)$$

where j is the time index, $t = j\Delta t$, and Δt is the time step.

(i) The input oxygen mole fraction x_i to the breathing plenum is found from bed 1 at $z = L$ or bed 2 at $z = 0$ depending on which bed has higher pressure. The mole fraction from the higher pressure bed is computed as C_A/C. This input mole fraction is used with equation (9) and the breathing flow W'_{BR} to solve for the output mole fraction, x_0. Equation (9) is solved as two coupled ordinary differential equations via a simple Euler method.

(iii) March in time by proceeding to step (i) for the new time level.

The time step and space lumps were chosen by performing numerical experiments to insure accuracy and stability of the solution procedure. The model simulation time is approximately twice that of real time when computed on a CDC Cyber 750 150.

4 Comparison of Model With Experiment

The prototype experimental system is depicted in Figs. 1 and 2 The concentric molecular sieve beds have an inner area of 36.5 cm² and an effective outer area of 136. cm². The effective flow length of a bed is 39.4 cm. The beds are loaded with Linde 5A sorbent with zeolite particles of approximately 340 to 833 microns in diameter. The void fraction of the beds is $\epsilon = 0.3$. All experiments were run at room temperature of 24°C No noticeable variation in temperature was observed during the system operation which implies the isothermal assumption is valid for the system under study. The fully open supply pressure valve has an effective diameter of .78 cm. and a discharge coefficient of 0.8 The fully open exhaust pressure valve has an effective diameter of 1.12 cm and a discharge
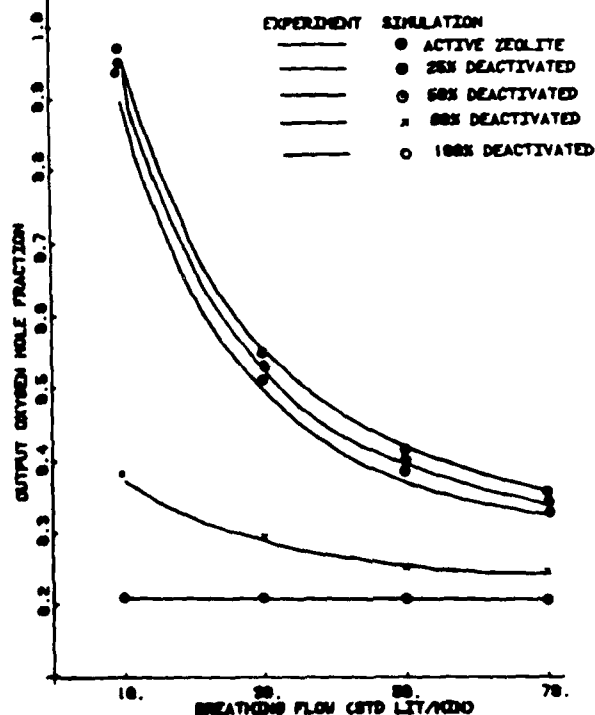
coefficient of 0.8. The purge orifice has a diameter of 0.191 cm and a discharge coefficient of 0.75. The breathing plenum volume is .0018 m³ an additional volume of .0006 m³ is added to this quantity to account for mixing in the connections.

In this paper, comparison with of the model is made with three basic types of experiments: (1) transient startup, (2) cycle time variation, and (3) change of active volume of zeolite in the beds.

4.1 Transient Startup of OBOGS. Shown in Figs. 4 through 7 are the results from the experimental data and the simulation model for the OBOGS at initially atmospheric pressure, the rotary valves turned on at time = 0, a supply pressure of 0.31 Mpa, an exhaust pressure of .10 Mpa, and cycle time of 10.7 seconds. These data are shown for four different constant breathing flowrates of 0.214, 0.642, 1.07, and 1.50 gm/min (10, 30, 50, and 70 standard liters/min). As can be seen in these figures, the model does an excellent job of matching the transient experimental data for the breathing oxygen mole fraction over the range of breathing flowrates. The increased ripple in the data and simulation for increased flow is due to less time for complete mixing in the plenum as the breathing flow goes up. The model describes this effect very well.

These plots indicate a method for controlling the outlet mole fraction. This is desirable since both high and low oxygen mole fraction can cause physiological problems [12] to the aircraft crew. By dumping product gas to artificially increase the breathing flow, the outlet mole fraction can be lowered if too high. If the mole fraction is too low, product gas dumping can be decreased.

4.2 Effect of Cycle Time Variation. In Fig. 8, the experimental and simulation results for a variation in cycle time are shown. As can be seen, the model does a good job of describing changes in oxygen output with cycle time variation. The results in this figure also demonstrate a method for controlling the outlet oxygen. By simply varying the cycle time of the process, control of oxygen output is possible. The cycle

time variation can be easily implemented by using a variable speed drive for the rotary valve. This control scheme has the advantage of not using any extra product gas which might be desirable for the contaminant filtering properties of the beds. The study of this control scheme is the subject of ongoing research and these results will be presented at a later date.

4.3 Bed Volume Variation. Figure 9 shows the effect of changing the volume of the beds, this was done experimentally [13] by filling the beds with fractional amounts of molecular sieve which had been deactivated with water. From simulation results, it was found that only bed volume and not shape is of importance for oxygen output. This might be an important design result, for it implies that the shapes of the beds are not critical. This means that the beds could be shaped for space considerations in the aircraft.

Another interesting result, is the relative insensitivity of the beds to volume changes until a critical volume is reached (around 75 percent for these beds). This also has important design implications. It means that sizing the system for increased flow is not just a simple increase in bed size, but a combination of volume changes and other design parameters. In particular, the valve areas and discharge coefficients are important design values.

In addition, these results indicate a potential problem in operation. If the beds were to become contaminated with water, which has the effect of decreasing the effective volume of the beds, there would be no outward indication of performance degradation until a critical volume were reached, and at that point the beds would rapidly lose performance with any further contamination.

5 Conclusions

A relatively simple model of a pressure swing oxygen generation system was developed in this study. The computerized model includes the zeolite beds, valves, and plenum breathing chamber in the system. The model predictions compare favorably with detailed experimental data. Ongoing work in this area include the prediction of temperature and contaminant effects and control of output breathing oxygen.

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APPENDIX C

COMPUTER MODEL FLOWCHART

I. Governing Equations

$$(1) \quad \frac{\partial(UC)}{\partial Z} = \beta(\gamma - C) \qquad\qquad \beta \equiv \frac{d - (1 - \varepsilon)}{\varepsilon}$$

$$(2) \quad \frac{\partial(UC_A)}{\partial Z} = \beta(\gamma_A - C_A) \qquad\qquad \eta \equiv \eta_A + \eta_B$$

$$(3) \quad \frac{\partial \eta_A}{\partial t} = -d(\gamma_A - C_A) \qquad\qquad \gamma \equiv \gamma_A + \gamma_B$$

$$(4) \quad \frac{\partial \eta}{\partial t} = -d(\gamma - C)$$

$$(5) \quad \frac{\partial C}{\partial Z} = 0$$

$$(6) \quad W = C_d A \sqrt{\frac{2k}{R(k-1)}} \frac{P_u}{\sqrt{T}} \left[\frac{P_d}{P_u}\right]^{1/k} \sqrt{1 - \left[\frac{P_d}{P_u}\right]^{\frac{k-1}{k}}}$$

II. Procedures

(1) Initial guess P(1) and P(2)

(2) Use adsorption isotherms to calculate γ_A and γ_B

(3) Integrate equation (1) to get C:

$$(U_1 A_0 - U_0 A_1) C = \beta \int (\gamma - C)\, dz$$

$$C = \frac{1}{(U_1 A_0 - U_0 A_1)} \beta \int (\gamma - C)\, dz$$

(4)
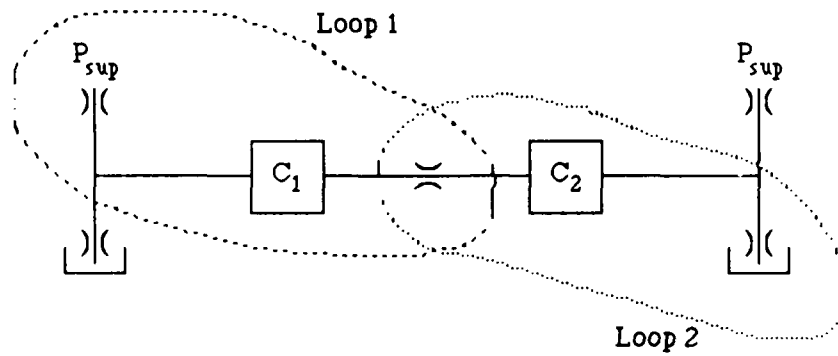
In Loop 1 and Loop 2, use False Position Method to find C_1 and C_2 so that these

values will be consistent with the supply pressure and exhaust pressure at each time step.

(5) Substitute P(1) and P(2) (calculated in step 4) into the valve eq. can get w(1), w(2), and w(3)

(6) Since Ui = W / (C1*Ai*Mi), where Mi is the molecular weight, U_{o1}, U_{l1}, and U_{o2} and U_{l2} can be calculated.

(7) Assume velocity is linear along the bed length. By integrating eq. (2), CA(Z) can be obtained.

(8) Use eq. (3) and eq. (4) to get new values for η_A, η_B and η for each time step.

(9) T = T + dT.
    Get a new valve area and repeat the procedure again.

III. Flowchart of the computer program

(1) Sign Convention
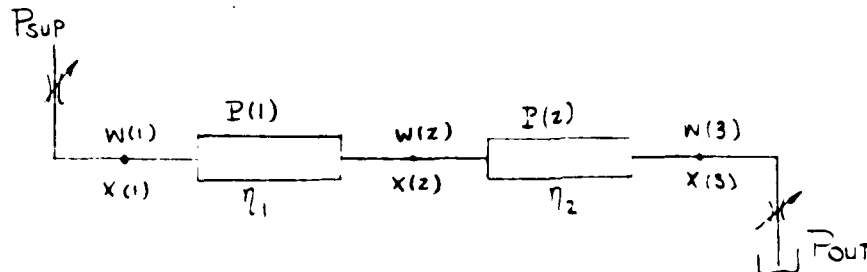
(2) Flowchart

    Please see attached.

START

CALL TIMEF

CALL BEDS — update time to calculate new n_A and n

CALL INITIAL — sets initial values for P(1),P(2), w(1),w(2), w(3),x(1),x(2),x(3), n1 and n2

CALL CONCEN — solves for w(1), w(2),w(3), P(1),P(2), U_{01}, $U_{\ell 1}$, U_{02}, and $U_{\ell 2}$
where U_{01} and $U_{\ell 1}$ are the velocities at the end of bed #1. U_{02} and $U_{\ell 2}$ are referred to bed #2.

CALL CONCA — solves for velocity distribution, $U(Z,t)$, and mole fraction $CA(Z,t)$ of each bed

is output option=4? — yes → write XA(1), XA(2), and ReGIS plotting commands to the graphics file

no

on-line ReGIS plotting for XBR, and w's

$T - TF$?

no

yes

STOP

program returns to the MENU and is ready for the next run

The inputs to the program are, as in the menu:

SYSTEM PARAMETERS

1. supply pressure	=	40.00	PSIA
2. outlet pressure	=	15.00	PSIA
3. final observation time	=	30.00	SEC.
4. cycle time	=	10.70	SEC.
5. breathing flowrate	=	10.00	STD LIT/MIN

GEOMETRIC PARAMETERS

6. by-pass valve diameter	=	0.0750	IN.
7. supply valve diameter	=	0.3062	IN.
8. outlet valve diameter	=	0.4387	IN.
9. bed length	=	15.50	IN.
10. outer bed diameter	=	5.7300	IN.
11. inner bed diameter	=	2.1800	IN.

BED PARAMETERS

12. KA	=	0.1530	KGMOLE O2 ABSORBED/KGMOLE GAS
13. KB	=	0.0490	KGMOLE N2 ABSORBED/KGMOLE GAS
14. B	=	2.6500	
15. diffusion coefficient	=	200.00	1/SEC
16. void fraction	=	0.37	

The user has the following options after he has reviewed the menu:

  1. change parameters
  2. insert a step change in the breathing flowrate, or
  3. exit the program

First, changing the parameters is done by entering the corresponding parameter number appeared in the menu. The program then prompts, for example:

ENTER THE PARAMETER AND PRESS "RETURN"

                                         CURRENT VALUE

SUPPLY PRESSURE (PSIA)   40.00

Once the new value has been assigned, the program goes back to the menu with modified parameter(s) and waits for the next input.

If, on the other hand, the user wishes to insert a step change in breathing flowrate, he enters the number for that option (which is "59" in this program). The program will ask for the starting and ending time, as well as the value for the step change and again goes back to the menu.

After the completion of modifications on the parameters, the user enters "0" to run simulation. The program responds with:

APPENDIX C

THE FOLLOWING PLOTS ARE AVAILABLE TO YOU ON THE TERMINAL

1   MOLE FRACTION OF OXYGEN VS.TIME (DATA FILE=MOLEFRAC.DAT)
2   INLET MASS FLOWRATE VS. TIME (DATA FILE=FLOWRATE.DAT)
3   OUTLET MASS FLOWRATE VS. TIME (DATA FILE=FLOWRATE DAT)
4   A DYNAMIC SIMULATION FOR ONE CYCLE (OXYGEN VS. TIME,
    DATA FILE=PROFILE.DAT)

PRESS THE CORRESPONDING # TO HAVE THE OUTPUT SHOWN AS THE
SIMULATION TRANSPIRES

The user chooses the desired output, and the program gives the following:

1   ENTER "0" TO RUN SIMULATION.
2   ENTER "19" TO CHANGE THE PARAMETERS
3   ENTER "99" TO EXIT PROGRAM.

ENTER THE CORRESPONDING # AND PRESS "RETURN"

and waits for the decision from the user. That is, it is still possible for
the user to go back to the menu before he runs the simulation.

Finally, the program asks for a last item:

DO YOU WISH TO DOUBLE THE NUMBER OF SPACE LUMPS IN
THE SIMULATION FOR BETTER ACCURACY ? (CURRENT NUMBER USED
IS 50) (Y/N)

This is due to the fact that when using one hundred lumps the
simulation is time consuming for the low breathing flowrate cases
The default is thus set to be 50 for faster simulation

APPENDIX C

```
CURRENT SYSTEM PARAMETERS ARE:
 1  SUPPLY PRESSURE=              40.00  PSIA
    OUTLET PRESSURE=             15.00  PSIA
    FINAL OBSERVATION TIME=      30.00  SEC
 4  CYCLE TIME=                  10.70  SEC
    BREATHING FLOWRATE=          10.00  STD LIT/MIN
 CURRENT GEOMETRIC PARAMETERS ARE:
    BY-PASS VALVE DIAMETER =    0.0750  IN
    SUPPLY VALVE DIAMETER =     0.3062  IN
 8  OUTLET VALVE DIAMETER =     0.4387  IN
 9  BED LENGTH =               15.5000  IN
10  OUTER BED DIAMETER =        5.7300  IN
11  INNER BED DIAMETER =        2.1800  IN
 THE CURRENT BED PARAMETERS ARE:
12  KA =                        0.1530  KGMOLES O2 ABSORBED/KGMOLE GAS
13  KB =                        0.0490  KGMOLES N2 ABSORBED/KGMOLE GAS
14  B =                         2.6500
15  DIFFUSION COEFFICIENT =    200.00  1/SEC
16  VOID FRACTION =             0.370
ENTER CORRESPONDING PARAMETER # TO CHANGE PARAMETER
ENTER "0" TO SIGNIFY PARAMETERS ARE CORRECT--RUN SIMULATION
ENTER "59" TO INSERT A STEP CHANGE IN BREATHING FLOWRATE
ENTER "99" TO EXIT PROGRAM
 1
```

```
++++++++++++***************************************************
```

```
ENTER THE PARAMETER AND PRESS "RETURN"
```

```
                                CURRENT VALUE
```

```
     PRESSURE (PSIA)              40.0000
```

APPENDIX C

```
 CURRENT SYSTEM PARAMETERS ARE
 1  SUPPLY PRESSURE=          30.00  PSIA
    OUTLET PRESSURE=          15.00  PSIA
 .  FINAL OBSERVATION TIME=   30.00  SEC
 ;  CYCLE TIME=               10.70  SEC
 .. BREATHING FLOWRATE=       10.00  STD LIT/MIN
  CURRENT GEOMETRIC PARAMETERS ARE:
 .. BY-PASS VALVE DIAMETER =  0.0750  IN
    SUPPLY VALVE DIAMETER =   0.3062  IN
    OUTLET VALVE DIAMETER =   0.4387  IN
    BED LENGTH =             15.5000  IN
 1. OUTER BED DIAMETER =      5.7300  IN
 1: INNER BED DIAMETER =      2.1800  IN
  THE CURRENT BED PARAMETERS ARE:
 1: KA =                      0.1530  KGMOLES O2 ABSORBED/KGMOLE GAS
 1. KB =                      0.0490  KGMOLES N2 ABSORBED/KGMOLE GAS
 1: B =                       2.6500
 1: DIFFUSION COEFFICIENT =   200.00  1/SEC
 1. VOID FRACTION =           0.370
ENTER CORRESPONDING PARAMETER # TO CHANGE PARAMETER
ENTER "9" TO SIGNIFY PARAMETERS ARE CORRECT--RUN SIMULATION
ENTER "59" TO INSERT A STEP CHANGE IN BREATHING FLOWRATE
ENTER "99" TO EXIT PROGRAM
59


****************************************************

ENTER THE TIME AT WHICH THE STEP CHANGE
IN BREATHING FLOWRATE IS TO OCCUR

THE FINAL OBSERVATION TIME IS CURRENTLY   30.00 SECONDS



1.




***************************************************

  .. THE TIME AT WHICH THE STEP CHANGE
  . BREATHING FLOWRATE IS TO END

  .. FINAL OBSERVATION TIME IS CURRENTLY   30.00 SECONDS
```

APPENDIX C

‡∷*∗*∗*∗∗**

ENTER THE NEW BREATHING FLOWRATE OCCURING AS
A STEP CHANGE FROM T=   10.00 TO T=   20.00 SECONDS

THE CURRENT BREATHING FLOWRATE IS 10.00 STD LIT/MIN

30

∶∣∗∤∗∤∗∗∗∗**

THE BREATHING FLOWRATE OF 30.00 STD LIT/MIN
WILL BE INPUT AS A STEP AT T=   10.00 SECONDS
AND WILL END AT T=   20.00 SECONDS

∶∗**************∗∗**

CURRENT SYSTEM PARAMETERS ARE:
```
 1   SUPPLY PRESSURE=              30.00  PSIA
 2   OUTLET PRESSURE=             15.00  PSIA
 3   FINAL OBSERVATION TIME=      30.00  SEC
 4   CYCLE TIME=                  10.70  SEC
 5   BREATHING FLOWRATE=          10.00  STD LIT/MIN
```
CURRENT GEOMETRIC PARAMETERS ARE:
```
 6   BY-PASS VALVE DIAMETER =  0.0750  IN
 7   SUPPLY VALVE DIAMETER =   0.3062  IN
 8   OUTLET VALVE DIAMETER =   0.4387  IN
 9   BED LENGTH =             15.5000  IN
10   OUTER BED DIAMETER =      5.7300  IN
11   INNER BED DIAMETER =      2.1800  IN
```
THE CURRENT BED PARAMETERS ARE:
```
12   KA =                     0.1530  KGMOLES 02 ABSORBED/KGMOLE GAS
13   KB =                     0.0490  KGMOLES N2 ABSORBED/KGMOLE GAS
14   K =                      2.6500
15   DIFFUSION COEFFICIENT =  200.00  1/SEC
16   VOID FRACTION =          0.370
```
ENTER CORRESPONDING PARAMETER # TO CHANGE PARAMETER
ENTER "0" TO SIGNIFY PARAMETERS ARE CORRECT--RUN SIMULATION
ENTER "59" TO INSERT A STEP CHANGE IN BREATHING FLOWRATE
ENTER "99" TO EXIT PROGRAM

APPENDIX C

THE FOLLOWING PLOTS ARE AVAILABLE TO YOU ON THE TERMINAL

1   MOLE FRACTION OF OXYGEN VS. TIME (DATA FILE=MOLEFRAC.DAT)
2   INLET MASS FLOWRATE VS. TIME (DATA FILE=FLOWRATE.DAT)
3   OUTLET MASS FLOWRATE VS. TIME (DATA FILE=FLOWRATE.DAT)
4   A DYNAMIC SIMULATION FOR ONE CYCLE (OXYGEN VS. TIME,
     DATA FILE=PROFILE.DAT)

PRESS THE CORRESPONDING # TO HAVE THE OUTPUT SHOWN AS THE
SIMULATION TRANSPIRES

1

1. ENTER "0" TO RUN SIMULATION.
2. ENTER "19" TO CHANGE THE PARAMETERS
3   ENTER "99" TO EXIT PROGRAM.
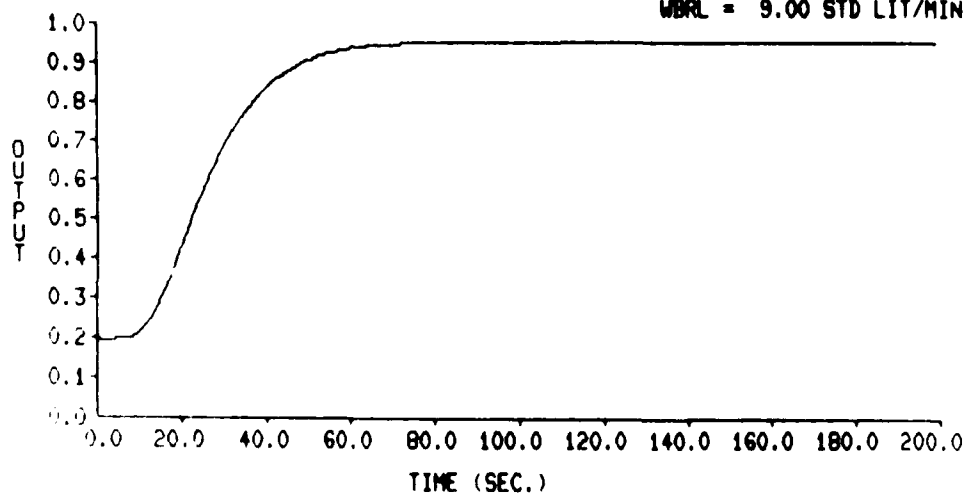
ENTER THE CORRESPONDING # AND PRESS "RETURN"

0

DO YOU WISH TO DOUBLE THE NUMBER OF SPACE LUMPS IN
THE SIMULATION FOR BETTER ACCURACY ? (CURRENT NUMBER USED
IS 50) (Y/N)

APPENDIX C

SAMPLE OUTPUTS

* OXYGEN MOLE FRACTION *

PSUP = 16.69 PSIA
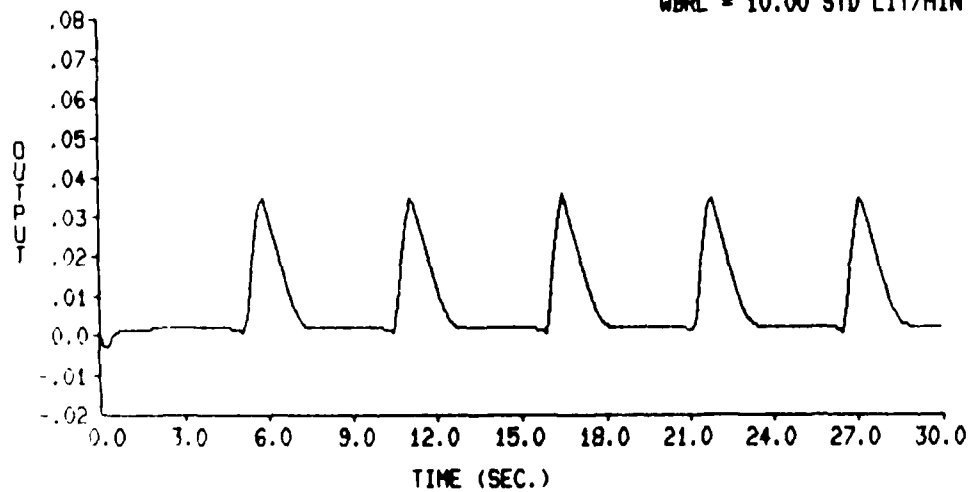POUT = 1.69 PSIA
WBRL = 9.00 STD LIT/MIN

PLEASE PRESS "C" TO CONTINUE :

APPENDIX C

SAMPLE OUTPUTS

INLET MASS FLOWRATE

PSUP = 40.00 PSIA
POUT = 15.00 PSIA
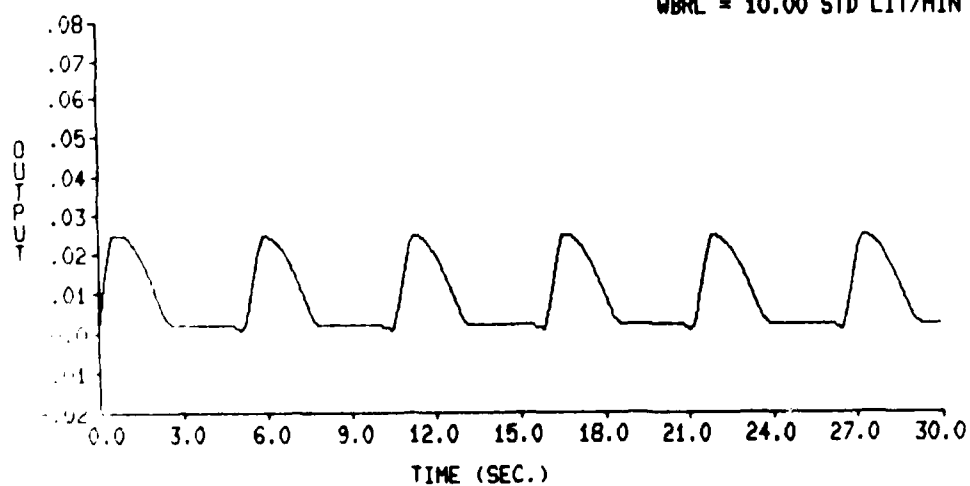WBRL = 10.00 STD LIT/MIN

PLEASE PRESS "C" TO CONTINUE :

APPENDIX C

SAMPLE OUTPUTS

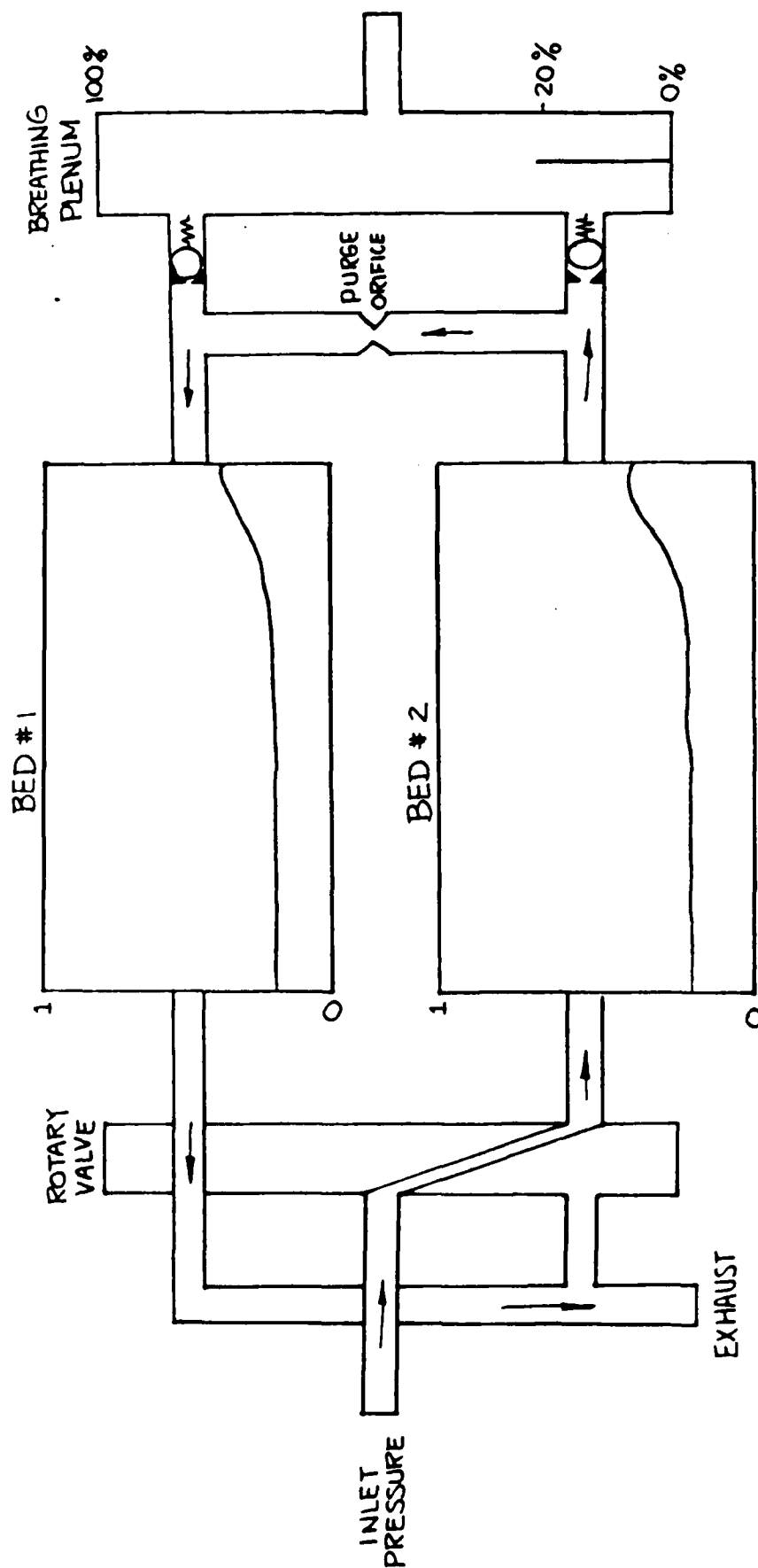* OUTLET MASS FLOWRATE (KG/SEC) *

PSUP = 40.00 PSIA
POUT = 15.00 PSIA
WBRL = 10.00 STD LIT/MIN

PLEASE PRESS "C" TO CONTINUE :

OBOGS SIMULATION

TIME = 7.0 SEC.

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